

Coherent Spin Dynamics into Space Quantization

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We propose a mechanism to describe how a physical quantity, which initially can take continuous values, is restricted within some discrete values after a measurement. As an example of the present theory, in which interplay between coherence of motion and fluctuation from disturbance plays an important role, we investigate motion of a spin state in a magnetic field. First, we point out that discrete eigenstates are formed from continuous states as a result of coherence of precession motion of a spin. Next, by assuming disturbance from environmental electromagnetic fields, we investigate temporal change of direction of a spin state by applying the first order perturbation theory and the Monte Carlo technique. Results of simulations show that the spins, whose directions are randomly distributed at the initial time, are reoriented toward only two directions due to fluctuation guided by coherence.

I. INTRODUCTION

In spite of the great success in a large number of applications, the quantum mechanics still contains a puzzling aspect in its foundations. One of the crucial questions is why and how an observed physical quantity is restricted within only some particular discrete values. A typical example is seen in the historical experiment achieved by O. Stern and W. Gerlach in 1922.[1, 2, 3] As is well known, they investigated trajectories of Ag atoms injected into an inhomogeneous magnetic field from a hot oven for the purpose of measuring momentum of Ag atoms. Contrary to naive expectation they observed split atom beams. This result indicated that magnetic momenta of the Ag atoms take only two values, even though the Ag atoms should have been randomly oriented when they escaped out of the hot oven. This effect, called space quantization, clearly exhibited that physical phenomena of atomic scale are essentially different from the concept of classical mechanics.

To date, the quantization effect is the foundation of the quantum mechanics which is the only reliable theory to describe physics of atomic scale. The quantization effect is often attributed to reduction of wavefunction which cannot be deduced from other principles. It is sometimes said that a measurement always causes the system jumps into an eigenstate of the measured variable. In spite of a number of theoretical trials to describe the reduction of a wavefunction in terms of a density matrix, the problem is still controversial.[4, 5, 6, 7]

It has been long thought that such a problem is too academic and useless even if it is important as the foundation of the quantum mechanics. However, recent development of technologies has enabled us to observe phenomena which could be carried out only in a conceptual experiment. For example, some experiments of quantum information have revealed essential aspects of the quantum mechanics as a real substance.[9] Behavior of electrons in a mesoscopic system also needs essential quantum mechanical viewpoints.[10] In addition, there are proposals of quantum computer utilizing nuclear spins[11] or electron spins in a quantum dot.[?] Therefore, deeper insight for the quantum mechanics is required, and it is of great significance to investigate motion of an spin for development of novel devices as well as for basic physics.

In this letter, we propose a mechanism to explain how a

physical quantity is quantized into some discrete levels when an observation is carried out. In order to describe the quantization process, we study the effect of quantum coherence on motion of a physical quantity with an example of a spin in a magnetic field. In the precedent studies, we have shown that coherence of time-evolving electron wave gives rise to formation of quantized eigenstates with discrete eigenenergies.[13, 14] We have calculated time-dependent density of states which exhibits transformation from a continuous spectrum into discrete levels, however, we have not taken the effect of scattering into account. In this study we investigate the effect of collaboration of coherence and fluctuation due to inelastic scattering, and show how a value of physical quantity approaches one of discrete eigenvalues.

There are theories that dephasing due to interaction between a quantum and environment plays an important role in a measurement process.[6, 7, 8] The present study is based on the similar standpoint. However, as far as we know, there have been no studies that pointed out the importance of interplay of coherence and scattering.

II. THEORY

A. Formation of eigenstates due to coherence

We investigate motion of a spin in a magnetic field, and show how it is quantized owing to interplay between coherence of motion and fluctuation due to environmental disturbance.

Let us consider a spin in a uniform magnetic field applied along the z -axis. This is a similar situation to the Stern-Gerlach experiment (SGE). However, we note that the situation of this study is different from that of the SGE in some points. First, we treat electron spins instead of momenta of Ag atoms. Next, we consider a uniform magnetic field, instead of inhomogeneous field used in the SGE. Inhomogeneity is only necessary to change electron's position in accordance with a direction of a spin. It is thus sufficient to consider motion in a uniform field when we are interested in directions of the spin. It is not difficult to include spatial motion of an electron by using wavepacket wavefunctions.

We consider a spin which is oriented a (θ, φ) direction in

the polar coordinate at the initial time $t = 0$. This spin state is expressed by a wavefunction

$$|\theta, \varphi\rangle = \cos(\theta/2) e^{-i\varphi/2} |+\rangle + \sin(\theta/2) e^{i\varphi/2} |-\rangle, \quad (1)$$

where $|+\rangle$ and $|-\rangle$ are the eigenstates of the spin operator s_z as

$$s_z |\pm\rangle = \pm \frac{\hbar}{2} |\pm\rangle. \quad (2)$$

Since the Hamiltonian of the interaction between a spin and a magnetic field, $\mathcal{H} = (eB/m)s_z$, is a generator of a time-evolution operator, the spin state in a magnetic field shows precession around the z -axis with a frequency $\omega = eB/m$ as

$$\begin{aligned} |\theta, \varphi, t\rangle &= |\theta, \varphi + \omega t\rangle \\ &= \cos(\theta/2) e^{-i(\varphi + \omega t)/2} |+\rangle + \sin(\theta/2) e^{i(\varphi + \omega t)/2} |-\rangle. \end{aligned} \quad (3)$$

We introduce here a superposition of the spin wavefunctions in the precessing motion as

$$|\chi(\theta, \varphi, t)\rangle = \frac{1}{\sqrt{t}} \int_0^t dt' e^{iE_\theta t'/\hbar} |\theta, \varphi, t'\rangle. \quad (4)$$

In this equation E_θ is energy of the spin state in a magnetic field given by $E_\theta = \langle \theta, \varphi | \mathcal{H} | \theta, \varphi \rangle = eB\hbar \cos \theta / 2m$. $|\chi(\theta, \varphi, t)\rangle$ is a coherent superposition of wavefunctions over the history during the time $0 \sim t$. In other words, we may interpret the function $|\chi(\theta, \varphi, t)\rangle$ as afterimage of precessing spin. The function $|\chi(\theta, \varphi, t)\rangle$ has a physical meaning as a time-integrated probability amplitude, i.e., the probability of finding a state at the direction θ during the period $0 \sim t$.

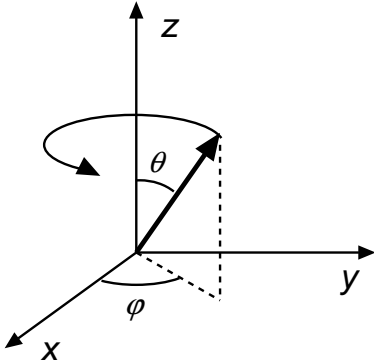


FIG. 1: Precession of a spin in a magnetic field applied along the z -axis.

We note that the exponential factor in eq. (4) has a role to cancel the time-dependent phase factor of $|\theta, \varphi, t'\rangle$, i.e., $e^{-iE_\theta t'/\hbar}$. This cancellation is important to obtain a rational result. Since we are considering a superposition of states belonging to different times, relative phase difference between the states changes if additional constant potential is applied. Thus the additional potential changes the superposed wavefunctions completely. Since such a situation is nonsense, the time-dependent phase factor should be excluded from the time-integration from the viewpoint of the gauge invariance of the superposed wavefunctions as shown in eq. (4).

By inserting eq. (3) into eq. (4), we can show that this function approaches the spin eigenstates with time as

$$\lim_{t \rightarrow \infty} |\chi(\theta, \varphi, t)\rangle \propto \begin{cases} |+\rangle & (\theta = 0) \\ |-\rangle & (\theta = \pi) \\ 0 & (\text{others}). \end{cases} \quad (5)$$

Eq. (5) means that we can interpret that eigenstates are formed as a result of coherence of motion of a precessing spin. When energy of the precessing spin coincides with one of eigenenergies $E_\pm = \pm eB\hbar/2m$, the coherent superposition approaches corresponding eigenstate. On the other hand, if energy is apart from any of eigenenergies, superposition of moving states decays due to destructive self-interference.

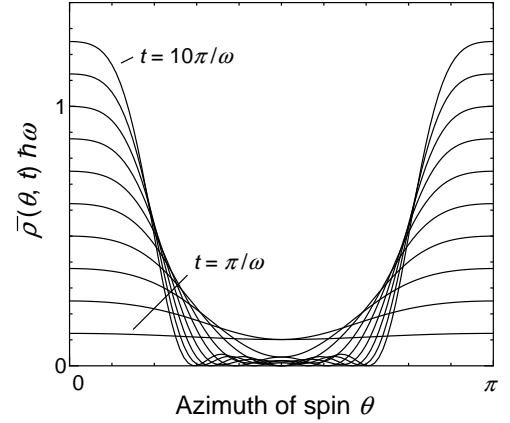


FIG. 2: The time-dependent density of states $\bar{\rho}(\theta, t)$ plotted as a function θ . Eash curve shows $\bar{\rho}(\theta, t)$ for the time $t = \pi/\omega \sim 10\pi/\omega$. Note that $\bar{\rho}(\theta, t)$ is normalized by a characteristic energy $\hbar\omega$.

In order to show how the continuous spectrum changes into discrete levels, we introduce a function $\bar{\rho}(\theta, t)$ with a norm of the function $\chi(\theta, \varphi, t)$ given by

$$\begin{aligned} \bar{\rho}(\theta, t) &= \frac{1}{2\pi\hbar} \langle \chi(\theta, \varphi, t) | \chi(\theta, \varphi, t) \rangle \\ &= \sum_{i=\pm} |A_i|^2 \delta_t(E_\theta \mp \hbar\omega/2). \end{aligned} \quad (6)$$

In this equation, $A_\pm \equiv \langle \theta, \varphi, 0 | \pm \rangle$ is an overlap integral between the initial state and the eigenstate. $\delta_t(E) = \sin^2(Et/2\hbar)/(\pi E^2 t/2\hbar)$ is the δ -function broadened due to finite lifetime. Since $\mp \hbar\omega/2$ are eigenenergies in a magnetic field we may interpret this function as density of states with broadened spectra due to finite lifetime formed as a result of coherent motion of a spin state.

Figure 2 shows $\bar{\rho}(\theta, t)$ normalized by a characteristic energy $\hbar\omega$ plotted as a function of θ . The curves show $\bar{\rho}(\theta, t)$ calculated for $t = \pi/\omega \sim 10\pi/\omega$. When t is small $\bar{\rho}(\theta, t)$ is an almost uniform function of θ . On the other hands, when t is large, $\bar{\rho}(\theta, t)$ has peaks around $\theta = 0$ and π . This means that probability to find the spin at the direction θ is restricted within the two values because of formation of eigenstates due to coherence. Considering that $|\chi(\theta, \varphi, t)\rangle$ is relevant to observation for finite duration of time, the behavior of $\bar{\rho}(\theta, t)$ means

we find a spin at any directions when t is small, whereas we find a spin only in the direction $\theta = 0$ or π in the long time.

B. Simulation of dynamics of spin direction

Let us presume that the direction of a spin fluctuates due to disturbance from environmental electromagnetic fields. Unfortunately, we lack detailed knowledge of the interaction between a spin and electromagnetic fields. We thus treat strength of the interaction as a parameter, and apply the first order time-dependent perturbation theory to investigate fluctuation of spin directions with a conventional picture of sudden change of spin directions.

We have to note that the set of the states $|\theta, \varphi\rangle$'s is overcomplete. In order to derive an expression of scattering probability with overcomplete basis including the effect of the coherence, we start from the Lippmann-Schwinger equation with the Born approximation

$$|\psi^+\rangle = |\theta, \varphi\rangle - \frac{i}{\hbar} \int_0^t d\tau e^{i(E_\theta - \mathcal{H})\tau/\hbar} V(\tau) |\theta, \varphi\rangle. \quad (7)$$

In this equation, $|\psi^+\rangle$ is a state generated from the initial state $|\theta, \varphi\rangle$ due to interaction between a spin and electromagnetic fields. We assume that the interaction is given by the operator $V(\tau) = V e^{\pm i\Omega\tau/\hbar}$ with Ω the frequency of the electromagnetic field. By inserting the completeness relation of the spin states

$$\frac{1}{2\pi} \int_0^\pi d\theta' \int_0^{2\pi} d\varphi' \sin\theta' |\theta', \varphi'\rangle \langle\theta', \varphi'| = 1 \quad (8)$$

into eq. (7), we have

$$|\psi^+\rangle \simeq |\theta, \varphi\rangle - \int_0^\pi d\theta' \int_0^{2\pi} d\varphi' \sin\theta' \times \left[\frac{iV}{2\pi\hbar} \int_0^t d\tau \langle\theta', \varphi'| e^{i(E_\theta - \mathcal{H} \pm \hbar\Omega)\tau/\hbar} |\theta, \varphi\rangle \right] |\theta', \varphi'\rangle. \quad (9)$$

This equation indicates that the scattered state $|\psi^+\rangle$ is written as a linear combination of spin states $|\theta', \varphi'\rangle$'s. Therefore, by following the ordinary argument of the time-dependent perturbation theory, we have the expression of scattering probability as

$$W(\theta', \varphi'; \theta, \varphi, t) \equiv \frac{|a_{\theta', \varphi'}(t)|^2}{t} = \frac{|V|^2}{2\pi\hbar} \rho(\theta', t), \quad (10)$$

where $a_{\theta', \varphi'}(t)$ is the quantity in the square bracket in eq. (9). $\rho(\theta', t)$ in this equation is given by an expression similar to eq. (6) but with different factors $B_+ = \cos(\theta/2) \cos(\theta'/2)$ and $B_- = \sin(\theta/2) \sin(\theta'/2)$ instead of A_\pm . We may regard $\rho(\theta', t)$ as time-dependent density of states for transition. Except the factor 2π arising from the prefactor of eq. (8), this expression is the same as the Fermi's golden rule. See ref. [14] for the detail of scattering theory with non-orthogonal overcomplete basis.

We investigated temporal change of spin directions by using the Monte Carlo simulation, taking stochastic nature of behavior of electrons into account.[15] The procedure of the simulation for a spin is

- (i) We set an initial direction of a spin with a random number. The spin begins precession.
- (ii) By considering that precession motion is interrupted due to inelastic scattering after time t_f , we evaluate t_f with an equation

$$-\log r_i = \int_0^{t_f} dt W(\theta, \varphi, t) \quad (11)$$

where r_i is another random number and

$$W(\theta, \varphi, t) = \int_0^\pi d\theta' \int_0^{2\pi} d\varphi' \sin\theta' W(\theta', \varphi'; \theta, \varphi, t) \quad (12)$$

is a total transition rate of the spin.

- (iii) We determine a new direction of the spin using a random number with weight given by $W(\theta', \varphi'; \theta, \varphi)$ which is evaluated from eq. (10).
- (iv) We repeat the steps (i), (ii), and (iii) considering that coherency is lost when inelastic scattering occurred, and accumulate relevant quantities.

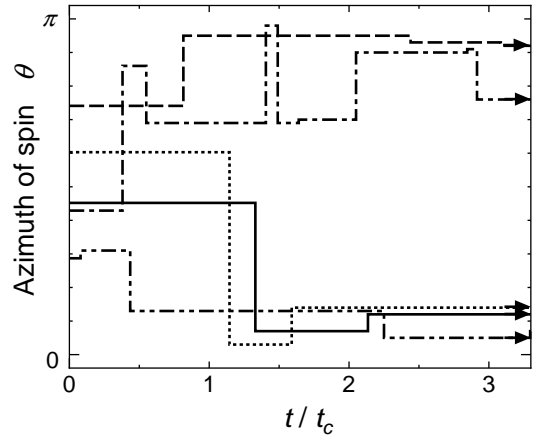


FIG. 3: Examples of spin motion calculated from the present theory. Sample paths calculated by the Monte Carlo simulations are plotted as functions time.

III. RESULTS AND DISCUSSION

Results of the Monte Carlo simulations are depicted in Figs. 3, 4 and 5. In Fig. 3, some of the sample paths (temporal change of azimuth of spins) calculated for the parameter $t_c/(2\pi/\omega) = 20$ are plotted as a function of time. The time is normalized by the characteristic time of scattering defined by $t_c \equiv 2\pi\hbar^2\omega/|V|^2$. An average interval of scattering events may be represented by t_c . As clearly shown in Fig. 3, the azimuth of spin fluctuates due to inelastic scattering, and approaches $\theta \simeq 0$ or π after receiving several scattering indifferent to the initial direction.

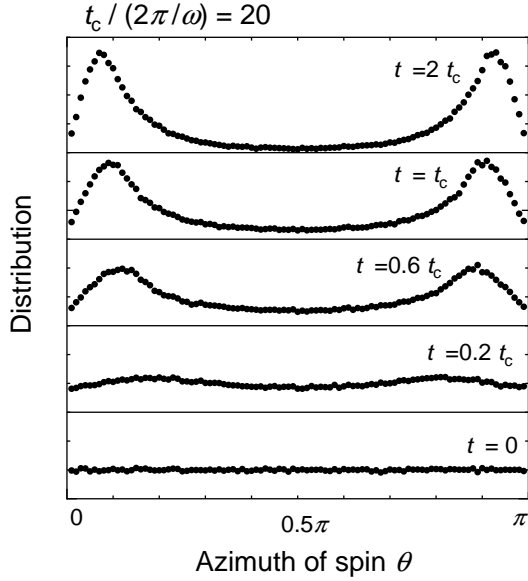


FIG. 4: Distribution of spin directions at the time $t = 0, 0.2t_c, 0.6t_c, t_c$ and $2t_c$ obtained from 100,000 paths of the Monte Carlo simulation with the parameter $t_c/(2\pi/\omega) = 20$.

Fig. 4 shows distribution of θ at the time $t = 0, 0.2t_c, 0.6t_c, t_c$ and $2t_c$ accumulated from 100,000 paths of the simulations. At the initial time $t = 0$, the azimuth distributes uniformly between 0 and π . With increasing time, the distribution curve shows two broad peaks corresponding to the most probable direction to be observed. This is because, as also shown in Fig.3, a spin is reoriented toward the two directions 0 or π while receiving scattering several times.

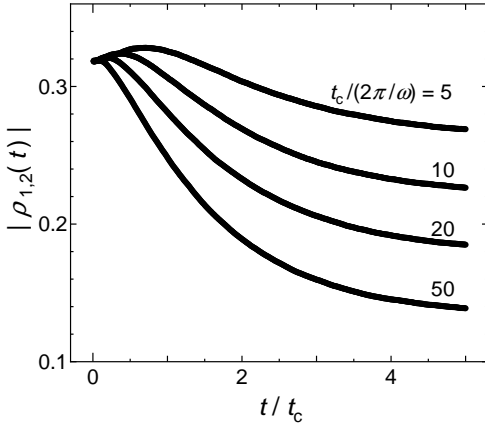


FIG. 5: The off-diagonal element $|\rho_{12}(t)|$ of the density matrix are plotted as a function of time.

This quantization effect arises from interplay between co-

herence of precession motion and fluctuation due to inelastic scattering. The transition probability is proportional to density of final states which is formed as a result of coherent superposition of moving spin states. Since the density of states has peaks around $\theta = 0$ and π , the final states tend to have these values of azimuth. This also means that there must be enough long time between scattering events for the coherence to be formed. When an interval of successive scattering events is very long, possible final states of scattering will be restricted to $\theta = 0$ or π . On the other hand, if scattering occurs very frequently, final states can have any directions. In other words, it is necessary that the ratio between scattering interval and precession period $t_c/(2\pi/\omega)$ must be large for this mechanism of quantization to occur.

We can interpret the quantization process in terms of phase coherency of an ensemble of spins. Properties of an ensemble is well expressed by a density matrix given by an average over N spins as

$$\rho_{m,n}(t) = \frac{1}{N} \sum_{j=1}^N |\theta_j, \varphi_j, t\rangle \langle \theta_j, \varphi_j, t|, \quad (13)$$

where j specifies each spin. Figure 5 shows the off-diagonal element of the density matrix evaluated from the simulations. With increasing time, the off-diagonal element decreases, indicating that the ensemble of spins approaches a mixed ensemble as $\rho_{m,n} \simeq (1/2)\delta_{m,n}$ due to reduction of phase coherency.

Finally we note that this theory can be verified in experiments. Even though the strength of inelastic scattering is unknown, we can vary the parameter t/t_c by changing length of the region where a magnetic field exists. It is also possible to change the parameter $t_c/(2\pi/\omega)$ by changing magnitude of the applied magnetic field. We expect that the distribution curves of spin direction as shown in Fig. 4 will be obtained from measurements with various conditions.

IV. CONCLUSION

In conclusion, we have proposed a mechanism to describe how a physical quantity is quantized due to an observation. We have shown that the interplay between coherence and fluctuation leads a spin toward one of eigenstates. Base on this theory, we carried out simulations for motion of spin under both a magnetic field and disturbance from environment. The results of simulations clearly showed that the direction of the spin tends to approach only two values $\theta = 0$ or π while receiving several scattering. The results elucidated that space quantization of a spin can be explained by the interplay between coherent motion and decoherence due to scattering.

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